

An invariant class of wave packets for the Wigner transform

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Abstract

Generalised Hagedorn wave packets appear as exact solutions of Schrödinger equations with quadratic, possibly complex, potential, and are given by a polynomial times a Gaussian. We show that the Wigner transform of generalised Hagedorn wave packets is a wave packet of the same type in phase space. The proofs build on a parametrisation via Lagrangian frames and a detailed analysis of the polynomial prefactors, including a novel Laguerre connection. Our findings directly imply the recently found tensor product structure of the Wigner transform of Hagedorn wave packets.

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1. Introduction

Hagedorn wave packets are prototypes of quantum wave functions that are highly localised in both, position and momentum space. They arrive as eigenstates of general multidimensional harmonic oscillators. The k -th wave packet, $k \in \mathbb{N}^d$, can be written as

$$\varphi_k(x) = p_k(x)g(x), \quad x \in \mathbb{R}^d,$$

where p_k is a polynomial of degree $|k|$ and g is a Gaussian with complex width matrix; see [10, 12, 18].

The favourable properties of Hagedorn wave packets have turned them into an essential tool for various applications, notably in molecular quantum dynamics and quantum optics. For instance, they have been used in the analysis of time-dependent semiclassical Schrödinger equations [11, 14, 17], the construction of numerical methods for high frequency problems [19, 6], and the representation of quasiprobabilities in quantum optics [21].

In the literature, Hagedorn wave packets also coexist as generalised squeezed states; see [2]. These states are generated by applying translation and squeezing operators to the eigenstates of the standard harmonic oscillator. However, this construction and Hagedorn’s approach produce, up to a phase factor, the same wave packets, see [18].

In this paper our aim is to analyse the representation of Hagedorn wave packets on phase space, that is, their Wigner functions, and give a comprehensive description of the appearing structures.

So far, Wigner functions have been classified for Hermite functions, see [7, 20], by using the well-known Hermite-Laguerre connection. This link has been generalised in [18], showing that the Wigner functions of a Hagedorn wave packet factorises regardless of the structure of the wave packet itself. Another approach using ladder operators in the two-dimensional setting can be found in [4].

Building on the generating function of the wave packets from [13], we are able to present a general formula for the Wigner functions of Hagedorn wave packets. As our main result, in Theorem 11 we show that the wave packets in phase space are given by Hagedorn wave packets of doubled dimension. This insight allows to lift all qualities of the wave packets to phase space and, thus, enables new perspectives and approaches in modelling and approximation theory. We find that the structure of the Wigner functions can be explained with the properties of the wave packets. A connection between the polynomial prefactor in the Wigner functions and Laguerre polynomials then reproduces the previously found factorisation results.

Wigner functions play a central role in microlocal analysis and semiclassical quantum mechanics; see, e.g., [3, 22]. In particular, various important semiclassical approximations and algorithms for the simulation of quantum molecular dynamics combine the Wigner function of the initial state with classical dynamics on phase space, see, e.g., [1, 16, 8]. Our results can contribute to improving these methods by providing new methods for the approximation of Wigner functions of more general states, and extending the applicability of wave packet propagation methods to phase space.

1.1. Outline

Motivated by the form the wave packets attain under non-unitary time evolution, in Chapter 2 we start with a generalised definition for Hagedorn wave packets; see also [17]. For our analysis we follow a geometric approach based on Lagrangian frames. However, all conditions can easily be translated into the classical ones found in [19] or [12].

In order to find criterions for tensor factorisation, in Chapter 3 we analyse the polynomial prefactors p_k of the wave packets. We characterise these poly-

nomials by a three-term recursion relation, a generating function as well as a ladder operator. All definitions are closely related to the corresponding formulas for Hermite polynomials, and thus suggest an interpretation as multivariate Hermite polynomials. However, the polynomials are not simple tensor products of univariate Hermite polynomials, but generically exhibit a more complex structure, as shown in Proposition 8. Nevertheless, our findings can be read as reasonable multivariate extension of the relations between Hermite and Laguerre polynomials discussed in [20].

In Chapter 4, we use the generating function to identify the Wigner function of Hagedorn wave packets with a wave packet of doubled dimension. This result combined with our polynomial analysis from Chapter 3 give a detailed picture of Hagedorn wave packets in phase space that constitutes the core of our manuscript.

Finally, in Chapter 5, we illustrate characteristic examples for both, polynomials and wave packets in two dimensions.

2. Generalised Hagedorn wave packets

In this chapter we adopt the viewpoint of [17], and briefly sketch the geometric approach to defining Hagedorn wave packets. Moreover, we extend this framework by decoupling the raising operator from the ground state. This type of generalised wave packets appears for example in the context of non-selfadjoint evolution problems, see [15, 9, 17].

2.1. Lagrangian frames and ground states

We consider the classical phase space $T^*\mathbb{R}^d = \mathbb{R}^{2d}$, equipped with the standard symplectic form

$$\Omega = \begin{pmatrix} 0 & -\text{Id}_d \\ \text{Id}_d & 0 \end{pmatrix} \in \mathbb{R}^{2d \times 2d}.$$

Definition 1. *A matrix $Z \in \mathbb{C}^{2d \times d}$ is called a Lagrangian frame, if*

$$Z^T \Omega Z = 0 \tag{1}$$

and $\text{rank } Z = d$. Furthermore, Z is called normalised, if

$$\frac{i}{2} Z^* \Omega Z = \text{Id}_d. \tag{2}$$

In the following, we will denote typical phase space points by $z = (q, p) \in \mathbb{R}^{2d}$, with $q \in \mathbb{R}^d$ being the position, and $p \in \mathbb{R}^d$ the momentum variable. Similarly, we write $Z = (Q; P)$ with $Q, P \in \mathbb{C}^{d \times d}$ for Lagrangian frames. With this denotation, the isotropy condition (1) and the normalisation condition (2) coincide with the symplecticity condition in [19] or, by taking $Q = A$ and $P = iB$, with Hagedorn's original definition in [12].

The image of a normalised Lagrangian frame Z is a complex Lagrangian subspace range $Z \subset \mathbb{C}^{2d}$. All Lagrangian frames spanning the same subspace L are related by unitary transformations, see, e.g., [17, §2.1], and thus have the same Hermitian square ZZ^* . Hence, considering the matrix

$$G_Z = \Omega^T \operatorname{Re}(ZZ^*) \Omega = \begin{pmatrix} PP^* & -PQ^* + i\operatorname{Id}_d \\ -QP^* - i\operatorname{Id}_d & QQ^* \end{pmatrix} \quad (3)$$

is a convenient way to classify the Lagrangian subspace range Z . The matrix G_Z is real, symmetric, positive definite and symplectic, and thus called the symplectic metric associated with the Lagrangian subspace range Z . The matrix G_Z plays an important role when lifting the wave packets to phase space.

Following the idea of Hagedorn, we can associate a coherent ground state with any normalised Lagrangian frame.

Lemma 2 (Ground state). *Let $Z = (Q; P)$ be a normalised Lagrangian frame. Then, Q and P are invertible and*

$$\operatorname{Im}(PQ^{-1}) = (QQ^*)^{-1} > 0.$$

In particular, for $\varepsilon > 0$,

$$\varphi_0^\varepsilon[Z](x) = (\pi\varepsilon)^{-\frac{d}{4}} \det(Q)^{-\frac{1}{2}} \exp\left(\frac{i}{2\varepsilon} x^T PQ^{-1}x\right) \quad (4)$$

is a square integrable function with $\|\varphi_0^\varepsilon[Z]\|_{L^2} = 1$.

A rigorous proof of this result can for example be found in [19]. Briefly, isotropy (1) ensures $\varphi_0^\varepsilon[Z] \in L^2(\mathbb{R}^d)$, while $\varphi_0^\varepsilon[Z]$ is normalised if and only if Z is normalised.

2.2. Excited states and spectral properties

Let \hat{q} denote the position operator and \hat{p} the momentum operator. Analogously to phase space points, we write $\hat{z} = (\hat{q}, \hat{p})$. Using this notation, we can define a linear operator

$$A^\dagger[Y] = \frac{i}{\sqrt{2\varepsilon}} Y^* \Omega \hat{z} \quad (5)$$

associated with a normalised Lagrangian frame Y . The components of $A^\dagger[Y]$ commute due to the isotropy of Y . Starting from a ground state $\varphi_0^\varepsilon[Z]$, the generalised Hagedorn wave packets $\varphi_k^\varepsilon[Z, Y]$ then are constructed via $A^\dagger[Y]$ as follows.

Definition 3 (Generalised wave packets). *Let $k \in \mathbb{N}^d$ and $Z, Y \in \mathbb{C}^{2d \times d}$ be normalised Lagrangian frames. Then, the k -th Hagedorn wave packet is defined as*

$$\varphi_k^\varepsilon[Z, Y] = \frac{1}{\sqrt{k!}} (A^\dagger[Y])^k \varphi_0^\varepsilon[Z] \quad (6)$$

with standard multiindex notation, $(A^\dagger[Y])^k = A^\dagger[Y]_1^{k_1} \dots A^\dagger[Y]_d^{k_d}$.

Based on this definition we will refer to $A^\dagger[Y]$ as raising operator.

If $Y = Z$, the above definition yields the standard Hagedorn wave packets $\{\varphi_k^\varepsilon[Z]\}_{k \in \mathbb{N}^d}$ that form an orthonormal basis of $L^2(\mathbb{R}^d)$. In this case, the adjoint operator of $A^\dagger[Z]$,

$$A[Z] = -\frac{i}{\sqrt{2\varepsilon}} Y^T \Omega \hat{z}, \quad A_j[Z] \varphi_k^\varepsilon[Z] = \sqrt{k_j} \varphi_{k-e_j}^\varepsilon[Z],$$

plays the role of a lowering operator. This property does not hold for the generalised wave packets.

The construction of Hagedorn wave packets by means of $A^\dagger[Y]$ implies

$$\varphi_k^\varepsilon[Z, Y] = p_k^\varepsilon[Z, Y] \varphi_0^\varepsilon[Z],$$

where $p_k^\varepsilon[Z, Y]$, $k \in \mathbb{N}^d$, is a polynomial of total degree $|k|$.

Proposition 4. *Let $Z = (Q; P) \in \mathbb{C}^{2d \times d}$ and $Y = (X; K) \in \mathbb{C}^{2d \times d}$ be two normalised Lagrangian frames and $B = \frac{i}{2} Z^* \Omega Y$. Then, for $k \in \mathbb{N}^d$ it holds*

$$\varphi_k^\varepsilon[Z, Y](x) = \frac{1}{\sqrt{2^{|k|} |k|!}} q_k^M \left(\frac{1}{\sqrt{\varepsilon}} B^* Q^{-1} x \right) \varphi_0^\varepsilon[Z](x) \quad (7)$$

with $M = \frac{1}{4} Y^* G_Z \bar{Y} + B^* Q^{-1} \bar{Q} \bar{B}$ and the polynomials $\{q_k^M\}_{k \in \mathbb{N}^d}$ that are recursively defined by $q_0^M \equiv 1$ and

$$(q_{k+e_j}^M(x))_{j=1}^d = 2x q_k^M(x) - 2M \cdot (k_j q_{k-e_j}^M(x))_{j=1}^d.$$

In the special case $Y = Z$ we find $B = \text{Id}$ and $M = Q^{-1} \bar{Q}$.

Proposition 4 is easily proven by identifying the found raising operator with the recursive definition of $\{\varphi_k^\varepsilon\}_k$, see Appendix Appendix A. A similar result for special choices of Y can be found in [17]. Proposition 4 reveals that the structure of the Hagedorn wave packets can be understood by studying the polynomial prefactors $\{q_k^M\}_k$. This polynomial analysis is conducted in the next section.

In this chapter we only introduced wave packets centered at the origin. In general, one obtains wave packets centered at any phase space point $z = (q, p) \in \mathbb{R}^{2d}$ by applying the linear Heisenberg-Weyl operator

$$(T_z \psi)(x) = e^{ip^T(x-q/2)/\varepsilon} \psi(x-q)$$

to the corresponding wave packet centered at the origin.

Also in the remaining parts of this paper, we only present our analysis for the wave packets centered at the origin. However, we stress that all of our results and proofs easily adapt to the more general case.

3. Analysis of the polynomial prefactor

In this chapter we analyse the polynomial prefactors of Hagedorn's wave packets, which are defined for a symmetric and unitary matrix $M \in \mathbb{C}^{d \times d}$ via the three-term recursion relation (TTRR)

$$(q_{k+e_j}^M(x))_{j=1}^d = 2x q_k^M(x) - 2M \cdot (k_j q_{k-e_j}^M(x))_{j=1}^d, \quad (8)$$

see Proposition 4, where e_j denotes the j -th unit vector in \mathbb{R}^d with boundary conditions $q_0^M \equiv 1$ and $q_\ell^M \equiv 0$ for all $\ell \notin \mathbb{N}^d$. This recursion is well-defined as M is symmetric. Equivalently, the polynomials q_k^M could be defined via their generating function or raising operator, both of which we derive in this section.

Surprisingly, this class of polynomials seems to be little studied in the literature found by the authors. A notable exception is [5] who defined them through their generating function and showed a generalised Mehler formula. In [4] one can find results for the two-dimensional case.

3.1. Generating function and raising operator

To get an intuition, we quickly discuss the univariate polynomials first. In one dimension (8) simplifies to

$$H_{n+1}^\lambda(x) = 2xH_n^\lambda(x) - 2\lambda nH_{n-1}^\lambda(x)$$

with $\lambda \in \mathbb{R}$. Starting from $H_0^\lambda \equiv 1$ and $H_{-1}^\lambda \equiv 0$, for $\lambda = 1$ we produce the usual Hermite polynomials. For $\lambda \neq 0$ we find rescaled Hermite polynomials

$$H_n^\lambda = \lambda^{\frac{n}{2}} H_n^1 \left(\frac{x}{\sqrt{\lambda}} \right).$$

To complete the picture, for $\lambda = 0$, we generate monomials $H_n^0 = (2x)^n$.

In the multivariate case the polynomials may emerge as simple tensor products of Hermite polynomials, but typically attain a more involved structure. Recently, in [13], there has been published a formula for the generating function of (rescaled) polynomials of type (8).

Lemma 5 (Generating function). *Let $M \in \mathbb{C}^{d \times d}$ be symmetric and unitary. Then, the generating function of the polynomials $\{q_k^M\}_{k \in \mathbb{N}^d}$ is given by*

$$f(x, t) = \sum_{k \in \mathbb{N}^d} \frac{t^k}{k!} q_k(x) = \exp(2x^T t - t^T M t). \quad (9)$$

To give a more profound characterisation of the polynomials, we also look at the raising operator and the gradient formula for the polynomials q_k^M . In the language of Dirac ladders, the gradient plays the role of a lowering operator or annihilator for the polynomials.

Lemma 6 (Ladder operators). *Let $b_M^\dagger = 2x - M \nabla_x$ and $k \in \mathbb{N}^d$. Then, it holds*

$$(q_{k+e_j}^M)_{j=1}^d = b_M^\dagger q_k^M \quad \text{and} \quad \nabla q_k^M = 2(k_j q_{k-e_j}^M)_{j=1}^d. \quad (10)$$

Proof. The generating function satisfies $\nabla_x f = 2t f$ and

$$\nabla_t f = 2x f - M \nabla_x f = b_M^\dagger f.$$

By the definition of the generating function $f(x, t)$ it follows that

$$\partial_{t_j} f(x, t) = \sum_k \frac{t^{k-e_j}}{(k-e_j)!} q_k^M(x) = \sum_k \frac{t^k}{k!} q_{k+e_j}^M(x),$$

i.e. $\partial_{t_j} f$ simply shifts the summation index by one into the direction of e_j . The gradient formula then follows immediately from (8). \square

As a consequence of (8) and Lemma 6, the polynomials satisfy the Rodrigues formula

$$q_k^M(x) = \exp(x^T M^{-1}x) (-M\nabla)^k \exp(-x^T M^{-1}x). \quad (11)$$

3.2. Factorisation and eigenvectors

The structure of the multivariate polynomials q_k^M crucially depends on the matrix M in the TTRR (8). In fact, the polynomials q_k^M factorise for all $k \in \mathbb{N}^d$ if and only if their generating function factorises. We summarize this observation in the following remark.

Remark 7. By inspecting Lemma 5 one observes that the generating function of the polynomials $\{q_k^M\}_{k \in \mathbb{N}^d}$ factorises into m lower-dimensional generating functions of the same type if and only if there is a relabeling of the coordinates such that M is block diagonal with m blocks. In this case, the polynomials q_k^M are tensor products of m lower-variate polynomials of the same type for all $k \in \mathbb{N}^d$.

In particular, the polynomials q_k^M are tensor products of univariate polynomials for all k if M is diagonal. On the contrary, if M has nonzero offdiagonal entries, the polynomials q_k^M are not simple tensor products anymore.

The polynomials q_k^M form a set of simultaneous eigenvectors for the operators

$$T_j = \frac{(b_M^\dagger)_j \partial_{x_j} + \partial_{x_j} (b_M^\dagger)_j}{2} = (1 + 2x_j \partial_{x_j}) - \partial_{x_j} (M\nabla)_j, \quad j = 1, \dots, d,$$

acting, for example, on the space of polynomials on \mathbb{R}^d . This can easily be seen from

$$\begin{aligned} T_j q_k^M &= \frac{1}{2} \left((b_M^\dagger)_j 2k_j q_{k-e_j}^M + \partial_{x_j} q_{k+e_j}^M \right) \\ &= (2k_j + 1) q_k^M, \end{aligned}$$

similarly as in the computation of harmonic oscillator eigenvalues. Hence, q_k^M is an eigenvector belonging to the eigenvalue $2k_j + 1$ of T_j . Moreover, for $j \neq k$, the operators T_j and T_k commute if and only if $M_{jk} = M_{kj} = 0$. In other words, by the remark above, commutation of the operators reflects the factorisation of the polynomials.

3.3. Laguerre connection

As noted in Remark 7, the polynomials q_k^M factorise for all k if and only if M is block-diagonal. Therefore, our aim is to express the general polynomials as a linear combination of tensor products by deleting off-diagonal entries of M .

It turns out, that q_k^M can be rewritten as a Laguerre polynomial

$$L_n^{(\alpha)}(x) = \sum_{j=0}^n \binom{n+\alpha}{n-j} \frac{1}{j!} (-x)^j, \quad n \in \mathbb{N}, \quad \alpha \geq 0,$$

of the raising operators corresponding to the polynomials generated by a reduced matrix applied to 1. This generalised Laguerre connection adds a new point to the long list of relations between Hermite and Laguerre polynomials, see, e.g., [20]. More precisely, we express q_k^M via raising operators $b_{M[n,m]}^\dagger$, where $M[n,m]$ denotes the matrix M with deleted offdiagonal entries M_{nm} and M_{mn} , i.e.

$$(M[n,m])_{ij} = \begin{cases} 0, & \{i,j\} = \{n,m\}, \\ M_{ij}, & \text{otherwise.} \end{cases}$$

Proposition 8 (Laguerre connection). *Let $M \in \mathbb{C}^{d \times d}$ be symmetric, and $M_{nm} = \lambda \neq 0$ for some $n \neq m$. Suppose $k \in \mathbb{N}^d$ with $k_n \geq k_m$. Then,*

$$q_k^M(x) = \left(b_M^\dagger\right)^k 1 = (c^\dagger)^{k-k_m(e_n+e_m)} (-2\lambda)^{k_m} k_m! L_{k_m}^{(k_n-k_m)} \left(\frac{1}{2\lambda} c_n^\dagger c_m^\dagger\right) 1,$$

where $c^\dagger = b_{M[n,m]}^\dagger$ denotes the polynomial raising operator for the reduced matrix $M[n,m]$. The case $k_n < k_m$ is analogous.

Proof. Let f_M denote the generating function of the polynomials q_k^M derived in Lemma 5, and define $k[n,m] = k - e_n k_n - e_m k_m$. Then, one computes the series expansion in t as

$$\begin{aligned} f_M(x, t) &= f_{M[n,m]}(x, t) \exp(-2\lambda t_n t_m) \\ &= \left(\sum_{k \in \mathbb{N}^d} \frac{t^k}{k!} (c^\dagger)^k \right) \cdot (1 - 2\lambda t_n t_m + \frac{1}{2!} (2\lambda t_n t_m)^2 - \dots) \\ &= \sum_{k \in \mathbb{N}^d} \frac{t^k (c^\dagger)^{k[n,m]}}{(k[n,m])!} \left(\sum_{j=0}^{\min(k_n, k_m)} \frac{(-2\lambda)^j}{j!} \cdot \frac{(c_n^\dagger)^{k_n-j}}{(k_n-j)!} \cdot \frac{(c_m^\dagger)^{k_m-j}}{(k_m-j)!} 1 \right). \end{aligned}$$

Due to the definition of the generating function, this implies

$$q_k^M(x) = (c^\dagger)^{k[n,m]} \sum_{j=0}^{\min(k_n, k_m)} \frac{k_n! k_m! (-2\lambda)^j}{j! (k_n-j)! (k_m-j)!} (c_n^\dagger)^{k_n-j} (c_m^\dagger)^{k_m-j} 1 \quad (12)$$

and we can reorder the sum by means of the index $\ell = k_m - j \geq 0$, since $k_n \geq k_m$ holds by assumption. This finally leads to

$$\begin{aligned} q_k^M(x) &= (c^\dagger)^{k[n,m]} (-2\lambda)^{k_m} k_m! (c_n^\dagger)^{k_n-k_m} \sum_{\ell=0}^{k_m} \frac{k_n! (-\frac{1}{2\lambda} c_n^\dagger c_m^\dagger)^{k_m-\ell}}{(k_m-\ell)! (k_n-k_m+\ell)! \ell!} 1 \\ &= (c^\dagger)^{k[n,m]} (-2\lambda)^{k_m} k_m! (c_n^\dagger)^{k_n-k_m} L_{k_m}^{(k_n-k_m)} \left(\frac{1}{2\lambda} c_n^\dagger c_m^\dagger\right) 1, \end{aligned}$$

where we utilised that c_n^\dagger and c_m^\dagger commute. \square

A direct, illustrative consequence can be deduced for the two-dimensional case, for which

$$M = \begin{pmatrix} \lambda_1 & \lambda_3 \\ \lambda_3 & \lambda_2 \end{pmatrix} \quad \text{with } \lambda_1, \lambda_2, \lambda_3 \in \mathbb{C}.$$

Corollary 9. *Let $k \in \mathbb{N}^2$ with $k_1 \geq k_2$. Then,*

$$q_k^M(x) = \begin{cases} (-2\lambda_3)^{k_2} k_2! (a_{\lambda_1}^\dagger)^{k_1-k_2} L_{k_2}^{(k_1-k_2)} \left(\frac{1}{2\lambda_3} a_{\lambda_1}^\dagger a_{\lambda_2}^\dagger \right) 1, & \lambda_3 \neq 0, \\ (a_{\lambda_1}^\dagger)^{k_1} (a_{\lambda_2}^\dagger)^{k_2} 1, & \lambda_3 = 0. \end{cases} \quad (13)$$

The case $k_1 \leq k_2$ is analogous.

For the case $\lambda_3 = 0$, Equation (13) directly carries out to the factorisation

$$q_k^M(x) = H_{k_1}^{\lambda_1}(x_1) H_{k_2}^{\lambda_2}(x_2).$$

In the case $\lambda_3 \neq 0$, (13) guarantees that each q_k^M is just a linear combination of at most $\min\{k_1, k_2\}$ many tensor products of the form

$$(a_{\lambda_1}^\dagger)^n (a_{\lambda_2}^\dagger)^m 1 = H_n^{\lambda_1}(x_1) H_m^{\lambda_2}(x_2) \quad (14)$$

where $n - m = k_1 - k_2$ and $k_1 - k_2 \leq n \leq k_1$, $m \leq k_2$. Moreover, if $\lambda_1 = \lambda_2 = 0$, the diagonal creation operators a_0^\dagger produce monomials, and we obtain the formula

$$q_k^M(x) = (-\lambda_3)^{k_2} k_2! 2^{k_1} x_1^{k_1-k_2} L_{k_2}^{(k_1-k_2)} \left(\frac{2}{\lambda_3} x_1 x_2 \right) \quad (15)$$

whenever $\lambda_3 \neq 0$ and $k_1 \geq k_2$. See also §5.1 for illustrations.

We note that by applying Proposition 8 iteratively one obtains an expansion of the general polynomials q_k^M in terms of tensor product Hermite polynomials, see Appendix Appendix B.

4. Hagedorn wave packets in phase space

There are various representations of quantum systems on the classical phase space \mathbb{R}^{2d} . The most popular one is the Weyl correspondence, where suitable selfadjoint quantum observables $A : L^2(\mathbb{R}^d) \rightarrow L^2(\mathbb{R}^d)$ are represented by their semiclassical Weyl symbol $a : \mathbb{R}^{2d} \rightarrow \mathbb{R}$, and wave functions $\varphi, \psi \in L^2(\mathbb{R}^d)$ by their Wigner function

$$\mathcal{W}^\varepsilon(\varphi, \psi)(x, \xi) = (2\pi\varepsilon)^{-d} \int_{\mathbb{R}^d} \overline{\varphi}\left(x + \frac{y}{2}\right) \psi\left(x - \frac{y}{2}\right) e^{i\xi^T y/\varepsilon} dy. \quad (16)$$

Then, matrix elements of A can be computed via the phase space integral

$$\langle \varphi, A\psi \rangle_{L^2(\mathbb{R}^d)} = \int_{\mathbb{R}^{2d}} \mathcal{W}^\varepsilon(\varphi, \psi)(z) a(z) dz. \quad (17)$$

In this chapter our aim is to analyse the Wigner functions of Hagedorn wave packets. For readability, we write

$$\mathcal{W}_{k,\ell}^\varepsilon[Z, Y] = \mathcal{W}^\varepsilon(\varphi_k^\varepsilon[Z, Y], \varphi_\ell^\varepsilon[Z, Y])$$

for $k, \ell \in \mathbb{N}^d$, and regard (k, ℓ) as a multiindex in \mathbb{N}^{2d} . Note, that by invoking [3, Equation (9.25)] we could also allow two wave packets that have different phase space centers.

As our main result, we prove that the Wigner functions of Hagedorn wave packets on \mathbb{R}^d are given by related Hagedorn wave packets on the phase space \mathbb{R}^{2d} . For proving this invariance result, we first introduce a phase space lift of Lagrangian frames.

Lemma 10. *Let $Z = (Q; P) \in \mathbb{C}^{2d \times d}$ and $Y = (X; K) \in \mathbb{C}^{2d \times d}$ be two normalised Lagrangian frames and $B = \frac{i}{2} Z^* \Omega Y$. We define the lifted matrices as*

$$\mathcal{Z} = \begin{pmatrix} \mathcal{Q} \\ \mathcal{P} \end{pmatrix} = \begin{pmatrix} \frac{1}{2} \bar{Z} & \frac{1}{2} Z \\ \Omega \bar{Z} & -\Omega Z \end{pmatrix} \quad \text{and} \quad \mathcal{Y} = \begin{pmatrix} \mathcal{X} \\ \mathcal{K} \end{pmatrix} = \begin{pmatrix} \frac{1}{2} \bar{Y} & \frac{1}{2} Y \\ \Omega \bar{Y} & -\Omega Y \end{pmatrix}$$

in $\mathbb{C}^{4d \times 2d}$ with the symplectic form $\Omega_{4d} = \Omega \otimes \text{Id}_2$ on \mathbb{R}^{4d} . These have the following properties

1. \mathcal{Z} and \mathcal{Y} are normalised Lagrangian frames if and only if Z and Y are.
2. The symplectic metric fulfills $\mathcal{P} \mathcal{Q}^{-1} = 2iG_Z$.
3. For the lifted frames we have

$$\mathcal{B} = \frac{i}{2} \mathcal{Z}^* \Omega_{4d} \mathcal{Y} = \begin{pmatrix} \bar{B} & 0 \\ 0 & B \end{pmatrix}.$$

4. The lifted recursion matrix satisfies

$$\mathcal{M} = \begin{pmatrix} -\frac{1}{4} Y^T G_Z Y & (B^* B)^T \\ B^* B & \frac{1}{4} Y^T G_Z Y \end{pmatrix}.$$

5. For the special case $Y = Z$ it holds $\mathcal{B} = \text{Id}_{2d}$ and

$$\mathcal{M} = \mathcal{Q}^{-1} \bar{\mathcal{Q}} = \begin{pmatrix} 0 & \text{Id}_d \\ \text{Id}_d & 0 \end{pmatrix}.$$

Proof. For the first assertion, one computes

$$\mathcal{Y}^T \Omega_{4d} \mathcal{Y} = \begin{pmatrix} -\bar{Y}^T \Omega Y & 0 \\ 0 & Y^T \Omega Y \end{pmatrix}, \quad \mathcal{Y}^* \Omega_{4d} \mathcal{Y} = \begin{pmatrix} -\bar{Y}^* \Omega Y & 0 \\ 0 & Y^* \Omega Y \end{pmatrix},$$

and notes that \mathcal{Y} is normalised if and only if Y is.

One can easily prove that $\mathcal{Q}^{-1} = i\mathcal{P}^*$. Hence, the second part follows from

$$\mathcal{P} \mathcal{P}^* = (\Omega \bar{Z} - \Omega Z) \begin{pmatrix} -Z^T \Omega \\ Z^* \Omega \end{pmatrix} = -\Omega (\bar{Z} Z^T + Z Z^*) \Omega = 2G_Z.$$

The formula for \mathcal{B} is a direct computation. For the claimed form of \mathcal{M} first compute

$$\mathcal{Q}^{-1}\overline{\mathcal{Q}} = \frac{i}{2} \begin{pmatrix} -Z^T\Omega Z & -\overline{Z^*\Omega Z} \\ Z^*\Omega Z & \overline{Z^T\Omega Z} \end{pmatrix} = \begin{pmatrix} 0 & \text{Id}_d \\ \text{Id}_d & 0 \end{pmatrix}.$$

By calculating

$$\mathcal{Y}^T G_Z \mathcal{Y} = \mathcal{Y}^T \Omega_{4d}^T \mathcal{Z} \mathcal{Z}^* \Omega_{4d} \mathcal{Y} = \begin{pmatrix} -\overline{Y^T G_Z Y} & 0 \\ 0 & Y^T G_Z Y \end{pmatrix}$$

the claim follows. The last case follows from the isotropy condition under the additional assumption. \square

Since \mathcal{Z} is again a Lagrangian frame, we can lift all our previous results to the phase space and consequentially find a family of Hagedorn wave packets in doubled dimension. In order to avoid confusion, we denote Hagedorn wave packets on phase space by upper case letters $\Phi_{(k,\ell)}^\varepsilon$. In particular, a direct computation shows that

$$\mathcal{W}^\varepsilon(\varphi_0[Z])(z) = (\pi\varepsilon)^{-d} e^{-z^T G_Z z / \varepsilon} = (2\pi\varepsilon)^{-d/2} \Phi_{(0,0)}^\varepsilon[\mathcal{Z}](z), \quad (18)$$

see, e.g., [18]. For excited wave packets the following result holds true.

Theorem 11. *Assume that $Z, Y \in \mathbb{C}^{2d \times d}$ are normalised Lagrangian frames. Then, for $k, \ell \in \mathbb{N}^d$, the Wigner function $\mathcal{W}_{k,\ell}[Z, Y]$ is a Hagedorn wave packet on phase space,*

$$\mathcal{W}_{k,\ell}^\varepsilon[Z, Y] = (2\pi\varepsilon)^{-d/2} \Phi_{(k,\ell)}^\varepsilon[\mathcal{Z}, \mathcal{Y}].$$

Consequently, it holds

$$\mathcal{W}_{k,\ell}^\varepsilon[Z, Y](z) = \frac{(2\pi\varepsilon)^{-d/2}}{\sqrt{2^{|k|+|\ell|} k! \ell!}} q_{(k,\ell)}^\mathcal{M} \left(\frac{1}{\sqrt{\varepsilon}} \mathcal{B}^* \mathcal{Q}^{-1} z \right) \Phi_0^\varepsilon[\mathcal{Z}](z),$$

where the lifted matrices $\mathcal{Y}, \mathcal{Z}, \mathcal{Q}, \mathcal{P}, \mathcal{B}$, and \mathcal{M} have been defined in Lemma 10.

Proof. For the generalised Hagedorn wave packets, we find the generating function

$$\sum_{k \in \mathbb{N}^d} \frac{t^k}{\sqrt{k!}} \sqrt{2^{|k|}} \varphi_k^\varepsilon[Z, Y](x) = e^{\frac{2}{\sqrt{\varepsilon}} t^T B^* Q^{-1} x - t^T M t} \varphi_0^\varepsilon[Z](x) =: h_t(x) \quad (19)$$

by identifying the polynomial factors in Proposition 4. Note that h_t is a Gaussian function in x and t . By writing $z = (x, \xi)$ and $v = (t, s)$, we can easily compute the Wigner transformation of h_t and h_s as

$$\begin{aligned} \mathcal{W}^\varepsilon(h_t, h_s)(z) &= (2\pi\varepsilon)^{-d} \int_{\mathbb{R}^d} \overline{h_t(x + \frac{y}{2})} h_s(x - \frac{y}{2}) e^{i\xi^T y / \varepsilon} dy \\ &= (\pi\varepsilon)^{-d} e^{-z^T G_Z z / \varepsilon} e^{\frac{2}{\sqrt{\varepsilon}} v^T B^* Q^{-1} z + v^T M v}, \end{aligned}$$

where we identified the lifted matrices from Lemma 10.

Then, by formally interchanging the order of integration and summation, it is clear that

$$\mathcal{W}^\varepsilon(h_t, h_s)(z) = \sum_{k, \ell \in \mathbb{N}^d} \frac{t^k s^\ell}{\sqrt{k! \ell!}} \sqrt{2^{|k|+|\ell|}} \mathcal{W}_{k, \ell}[Z, Y](z),$$

which implies the result. For a rigorous justification, note that due to the Gaussian decay we can differentiate under the integral sign with respect to $v = (t, s)$. Evaluating the differentiated function at $v = (t, s) = (0, 0)$ then shows the result. \square

Remark 12. By invoking part (5) of Lemma 10, Theorem 11 explains the factorisation result for Hagedorn wave packets that has recently been discovered in [18]. Namely, the polynomial prefactor of $\mathcal{W}_{k, \ell}^\varepsilon[Z, Z]$ is a product of d polynomials,

$$\mathcal{W}_{k, \ell}^\varepsilon[Z, Z](z) = \frac{(2\pi\varepsilon)^{-d/2}}{\sqrt{2^{|k|+|\ell|} k! \ell!}} \Phi_0^\varepsilon[Z](z) \prod_{j=1}^d q_{(k_j, \ell_j)}^N \left(\left(\frac{1}{\sqrt{\varepsilon}} \mathcal{Q}^{-1} z \right)_j, \left(\frac{1}{\sqrt{\varepsilon}} \mathcal{Q}^{-1} z \right)_{d+j} \right),$$

where, for $k_j \geq \ell_j$ and $N = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$,

$$q_{(k_j, \ell_j)}^N(x_1, x_2) = (-1)^{\ell_j} \ell_j! 2^{k_j} x_1^{k_j - \ell_j} L_{\ell_j}^{(k_j - \ell_j)}(2x_1 x_2)$$

is a Laguerre polynomial of the form (15).

5. Examples

5.1. Polynomial prefactor

In order to illustrate different types of polynomials q_k^M , we present various examples for the nodal sets of two-dimensional polynomials $q_{i,j}^M$, for $(i, j) \in \mathbb{N}^2$. For simplicity, we restrict ourselves to real matrices M such that the polynomials generated by the TTRR (8) have real coefficients.

As examples we consider the unitary, symmetric matrices

$$M^{(1)} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad M^{(2)} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad M^{(3)} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}. \quad (20)$$

By recalling (14) and (15), the polynomial $q_{4,6}^{M^{(1)}}$ corresponds to a simple tensor product of one dimensional Hermite polynomials, while

$$q_{7,6}^{M^{(2)}} = 6! 2^7 x_1 L_6^{(1)}(2x_1 x_2). \quad (21)$$

One can see the consequences of these simple formulas in the structure of the nodal sets depicted in the upper panels of figure 1.

The matrix $M^{(3)}$ gives rise to a more complicated mixing between the two variables. This can also be seen from the illustration of $q_{6,5}^{M^{(3)}}$ in the lower panel of figure 1. It is striking that already for real matrices M in two dimensions the polynomials generated by the simple TTRR (8) develop such nontrivial nodal sets.

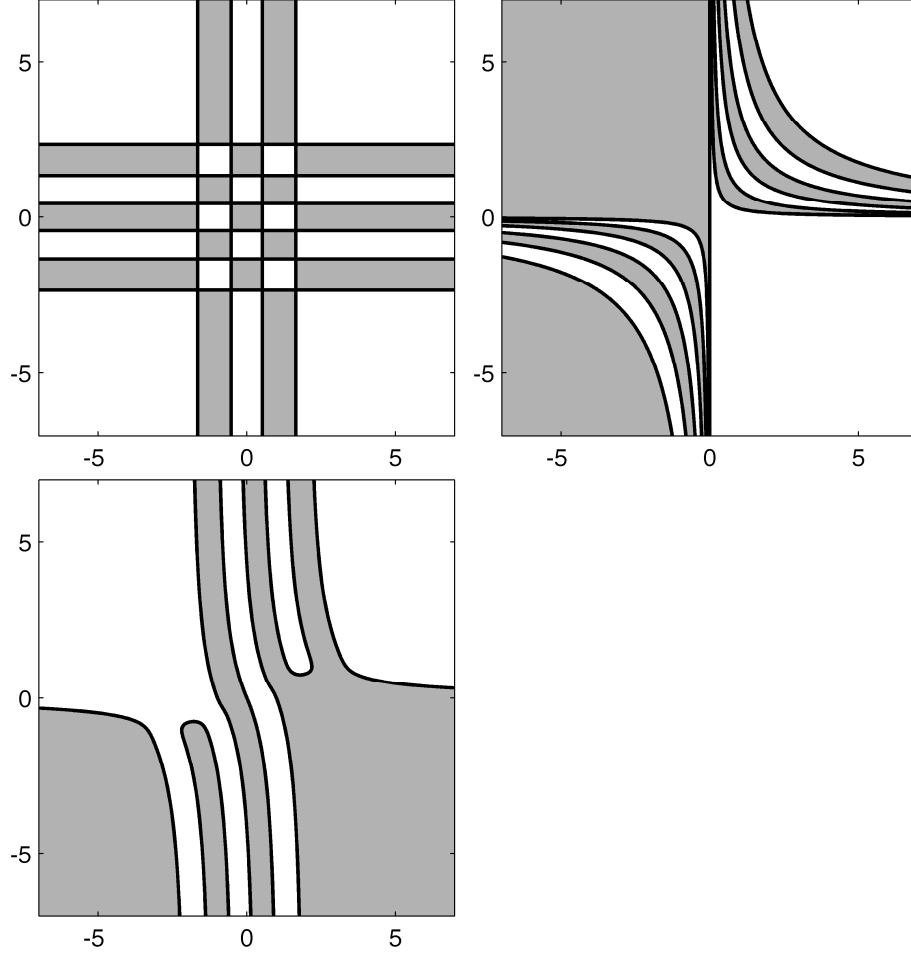


Figure 1: The nodal sets of three exemplary two-dimensional polynomials, associated with the matrices $M^{(1)}$ (upper left), $M^{(2)}$ (upper right) and $M^{(3)}$ (lower). Regions with negative values are highlighted by grey coloring.

5.2. Hagedorn wave packets

In this section we present two-dimensional examples of Hagedorn wave packets in order to indicate the variety of structures that can be realised.

For our illustrations we employ the same matrices $M^{(j)}$, $j \in \{1, 2, 3\}$ from (20) as used for the polynomials in §5.1. Our choice for the Lagrangian frames $Z_j = (Q_j; P_j)$ satisfying

$$Q_j^{-1} \overline{Q_j} = M^{(j)}, \quad j = 1, 2, 3,$$

is given by

$$Z_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \\ i & i \\ i & -i \end{pmatrix}, \quad Z_2 = \frac{1}{2} \begin{pmatrix} 1+i & 1-i \\ 1-i & 1+i \\ \frac{i-1}{2} & \frac{i+1}{2} \\ \frac{i+1}{2} & \frac{i-1}{2} \end{pmatrix}, \quad Z_3 = \begin{pmatrix} i & -i(1+\sqrt{2}) \\ 1 & \sqrt{2}-1 \\ \frac{1-\sqrt{2}}{2\sqrt{2}} & \frac{1}{2\sqrt{2}} \\ \frac{i+i\sqrt{2}}{2\sqrt{2}} & \frac{i}{2\sqrt{2}} \end{pmatrix}.$$

One can easily check that Z_1, Z_2 , and Z_3 are normalised Lagrangian frames.

We also consider an example of a generalised wave packet associated with the two Lagrangian frames Z_2 and Z_3 . In this case, the mixing matrix of the polynomials is given by the formula in Proposition 4 and does not equal $Q^{-1}\overline{Q}$.

We stress that despite the fact that the polynomials

$$q_k^{M_j}, \quad j = 1, 2, 3,$$

have real coefficients, the wave packets itself are not real-valued since the polynomials are evaluated on the subspace $Q_j^{-1}\mathbb{R}^d \subset \mathbb{C}^d$, which does not coincide with \mathbb{R}^d except for Z_1 . This case is very special, since one has

$$M = \text{Id} \iff Q \in \mathbb{R}^{d \times d},$$

which implies that the standard tensor Hermite polynomials q_k^{Id} appear only together with real transformations Q . Hence, all Hagedorn wave packets with $Q^{-1}\overline{Q} = \text{Id}$ correspond to rescaled, sheared, or shifted multivariate Hermite functions, while this is not true in the case $Q \notin \mathbb{R}^{d \times d}$.

Figure 2 displays the absolute value of two Hagedorn wave packets associated with the Lagrangian frames Z_1 and Z_2 . One can recognise that the Hagedorn wave packet $\varphi_{4,6}^{0,1}[Z_1]$ on the left hand side is just a rotated and rescaled Hermite function, as expected. In contrast, the wave packet $\varphi_{7,6}^{0,1}[Z_2]$ associated with $M^{(2)}$ has a circular structure, which arises due to a complex rotation of the hyperbolas from the upper right panel of figure 1.

For Z_3 the resulting wave packets exhibit complicated structures. The same is true for generalized wave packets associated with the two different Lagrangian frames Z_2 and Z_3 , as illustrated by the examples in figure 3.

For us, the variety of different Hagedorn wave packets is very fascinating. We suggest that the selective use of classes of Hagedorn wave packets with specific geometries could prove useful for designing meshfree numerical discretizations of evolution equations with a priori known symmetries.

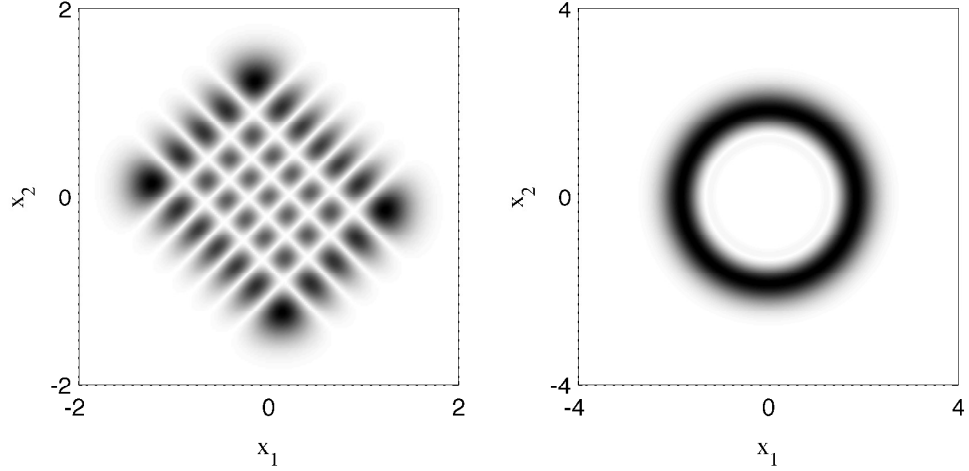


Figure 2: Intensity plot of the absolute value of the two exemplary two-dimensional Hagedorn wave packets $\varphi_{4,6}^{0,1}[Z_1](x)$ (left) and $\varphi_{7,6}^{0,1}[Z_2](x)$ (right), $\varepsilon = 10^{-1}$. Darker colouring represents higher absolute values.

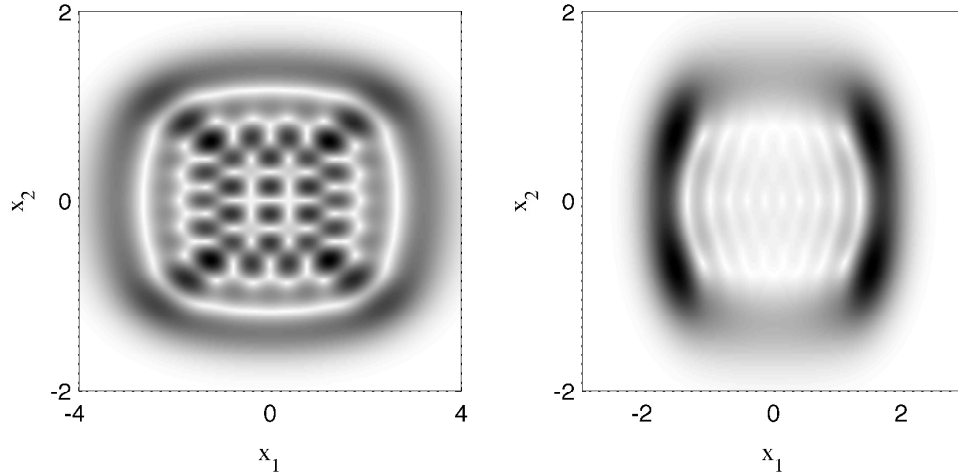


Figure 3: Intensity plot of the absolute value of the two-dimensional Hagedorn wave packets $\varphi_{6,5}^\varepsilon[Z_3](x)$ (left) and $\varphi_{3,7}^\varepsilon[Z_2, Z_3](x)$ (right), where $\varepsilon = 10^{-1}$.

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Appendix A. Proof of Proposition 4

Using the found structure of the polynomials q_k and the corresponding ladder operators, we can give a simple proof of Proposition 4.

Proof. We prove the assertion by induction over $|k|$. We know that the raising operator A^\dagger from (5) only creates polynomial prefactors in front of φ_0^ε . The idea is to rewrite A^\dagger as an operator acting on the prefactors only, and identifying it with the raising operator of the polynomials.

Since the case $k = 0$ is trivial, we assume the assertion to be true for some $k \in \mathbb{N}^d$. Then, for $j = 1, \dots, d$, by (6) we have

$$\begin{aligned} \varphi_{k+e_j}^\varepsilon[Z, Y](x) &= \frac{1}{\sqrt{k_j+1}} A_j^\dagger[Y] \varphi_k^\varepsilon[Z, Y](x) \\ &= \frac{2^{-\frac{|k|+1}{2}}}{\sqrt{(k+e_j)!}} \left(\frac{i}{\sqrt{\varepsilon}} [X^*(i\varepsilon \nabla_x - PQ^{-1}x) + K^*x]_j q_k^M \left(\frac{1}{\sqrt{\varepsilon}} B^* Q^{-1}x \right) \right) \varphi_0^\varepsilon[Z](x). \end{aligned}$$

Hence, the result is true as long as

$$q_{k+e_j}^M \left(\frac{1}{\sqrt{\varepsilon}} B^* Q^{-1}x \right) = [-\sqrt{\varepsilon} X^* \nabla_x + \frac{2}{\sqrt{\varepsilon}} B^* Q^{-1}x]_j q_k^M \left(\frac{1}{\sqrt{\varepsilon}} B^* Q^{-1}x \right),$$

which follows by invoking the polynomial raising operator of Lemma 6. It is easy to see that M is symmetric since the components of A^\dagger commute by the isotropy condition.

The structure of the matrix M follows from the fact that both $Q^{-1}\overline{Q}$ and QQ^* are symmetric and

$$B^* Q^* = \frac{i}{2} (K^* Q - X^* P) Q^* = \frac{i}{2} (K^* Q Q - X^* \overline{P} Q^T - 2i X^*)$$

since $PQ^* = (QP^* + 2i\text{Id})^T$. Hence,

$$\begin{aligned} B^* Q^* Q^{-T} \overline{B} &= \frac{i}{2} (K^* \overline{Q} \overline{B} - X^* \overline{P} \overline{B}) + X^* Q^{-T} \overline{B} = \frac{i}{2} Y^* \Omega \overline{Z} \overline{B} + X^* Q^{-T} \overline{B} \\ &= \frac{1}{4} Y^* \Omega \overline{Z} Z^T \Omega \overline{Y} + X^* Q^{-T} \overline{B} = -\frac{1}{4} Y^* \overline{G_{Z_0}} \overline{Y} + X^* Q^{-T} \overline{B}, \end{aligned}$$

where the last equality is due to the isotropy of Y . \square

Appendix B. Tensor product representation

By recursively applying Proposition 8, one can derive an expansion of the general polynomials q_k^M in terms of tensor products of univariate Hermite polynomials associated with the diagonal entries of M . Moreover, the required number of summands depends only on the number of offdiagonal entries of M for which $M_{ij} \neq 0$, and the corresponding indices k_i , and k_j .

Proposition 13 (Tensor product representation). *Let $M \in \mathbb{C}^{d \times d}$ be symmetric, and suppose that there are exactly $n \leq d(d-1)/2$ different off-diagonal index pairs $1 \leq \alpha_j < \beta_j \leq d$, $j = 1, \dots, n$, for which $M_{\alpha_j \beta_j} = \lambda_j \neq 0$. Then, for $k \in \mathbb{N}^d$,*

$$q_k^M(x) = \sum_{\substack{\ell \in \mathbb{N}^n \\ \ell_j \leq \min\{k_{\alpha_j}, k_{\beta_j}\}}} (-2\lambda)^\ell \ell! \binom{k_\alpha}{\ell} \binom{k_\beta}{\ell} \prod_{i=1}^d H_{k_i - (E\ell)_i}^{M_{i,i}}(x_i) \quad (\text{B.1})$$

with standard multiindex notation, e.g. $k_\alpha \in \mathbb{N}^n$ with $(k_\alpha)_j = k_{\alpha_j}$. The index matrix $E \in \mathbb{N}^{d \times n}$ is defined by

$$E_{ij} = (e_{\alpha_i} + e_{\beta_i})_j. \quad (\text{B.2})$$

Proof. We start by recalling (12), which can be rewritten as

$$q_k^M(x) = \sum_{m=0}^{\min\{k_{\alpha_j}, k_{\beta_j}\}} m! \binom{k_{\alpha_j}}{m} \binom{k_{\beta_j}}{m} (-2\lambda_j)^m q_{k-m(e_{\alpha_j}+e_{\beta_j})}^{M[\alpha_j, \beta_j]}(x) 1, \quad (\text{B.3})$$

for all $j = 1, \dots, n$. One can use the matrix E in order to write

$$k - m(e_{\alpha_j} + e_{\beta_j}) = k - (Em\hat{e}_j)$$

where \hat{e}_j denotes the j -th unit vector in \mathbb{R}^n . Iterating this procedure until all offdiagonal entries of M are deleted, completes the proof. \square

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